Kinetic Modeling of Styrene Epoxidation Reaction Catalyzed by Styrene Monooxygenase System

Seunghyuk Kim and Sunghoon Park
Department of Chemical and Biochemical Engineering, Pusan National University,
Busan 609-390, Korea
TEL: +82-51-510-3049, FAX: +82-51-517-2716

Abstract

Styrene monooxygenase (SMO), catalyzing styrene epoxidation reaction, is composed of two subunits, StyA and StyB. StyA, flavin-dependent monooxygenase component, converts styrene into (S)-styrene oxide by using one atom of oxygen. StyB, NADH-dependent reductase component, transfers the reducing equivalents from NADH to FAD. Reduced FAD ($FADH_2$) becomes the substrate of StyA. Therefore, SMO is classified as two-component flavin-diffusible monooxygenase family.[1] In order to identify the rate-limiting step and improve the specific styrene epoxidation rate of whole cell, a mathematical kinetic model of SMO was developed based on reaction mechanism for each subunit. It was assumed that StyA follows the kinetic mechanism of the hydroxylase subunit of methane monooxygenase and StyB follows random sequential binding kinetic model.[2),3)] Kinetic parameters were determined by using *in vitro* experimental results in the literature and the data-fitting program, Scientist® for Windows. The kinetic model could properly simulate SMO reaction kinetics obtained under most experimental conditions. Also, the model could determine the optimal concentrations of $FADH_2$ and NADH for the maximal SMO reaction rate when the volumetric reaction rates of StyA and StyB were given. The application of *in vitro* results to the development of whole-cell SMO biocatalyst is also discussed.

References

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